Search for Half-Metallic Magnetic Materials: Double Perovskites

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Introduction: The perovskite structure class, one of the most commonly occurring in all of materials science, has the general formula ABX_3, where A corresponds to a large electropositive cation, B represents a small transition metal, and X is generally an oxide or halide anion. Sr_2FeMoO_6 is an ordered double perovskite, with B-cations Fe^{3+} and Mo^{5+} (electron configurations $t_{2g}^3e_g^2$ and $t_{2g}^1e_g^0$, respectively), which undergoes a ferrimagnetic to metallic transition at approximately 420 K. Although these compounds are metallic, there is significant evidence that electron transport occurs via exchange of the Mo^{5+} d^1 electron. This transport is highly spin-polarized – the compound is only metallic when the conducting electron has an opposite spin than the Fe^{3+} d^5 electrons. A large inter-grain boundary resistance exists which can be significantly diminished through application of a magnetic field, thus giving this compound its magnetoresistant property.

In this study, the structural, magnetic, and transport properties of several double-perovskites (specifically, Sr_2MnMoO_6, $SrLaMnMoO_6$, Sr_2MnRuO_6, $SrLaMnMoO_6$, Sr_2VMoO_6 and Ca_2VMoO_6) were studied, in order to achieve a better comprehension of the relative energy levels of the B cations and magnetoresistant properties of these materials. To explain why these compounds lack or portray magnetoresistant properties, we used variable temperature high-resolution synchrotron X-ray and neutron powder diffraction techniques, electrical transport, and magnetic susceptibility measurements. Variable temperature high-resolution synchrotron X-ray measurements were taken to determine the structure-property relationship of the phase transitions.

Methods and Materials: Polycrystalline samples were prepared in air from stoichiometric quantities of $CaCO_3$, $SrCO_3$, MoO_3, V_2O_5, La_2O_3, and RuO_2 using conventional ceramic synthesis techniques. Initial annealing cycles were carried out in air in the 875 – 1100 ^oC range to decompose the carbonates. After a one hour purge, the molybdenum samples were heated in flowing H_2 (5%) / N_2 for 8 – 12 hours in the 1000 – 1250 ^oC. The ruthenium samples were heated in air with final anneal temperatures in the range of 1300 – 1450 ^oC. Magnetic susceptibility measurements were obtained using a SQUID magnetometer. Variable temperature high-resolution synchrotron X-ray measurements were taken at the X7A beamline. Electrical resistivities were measured on sintered pellets using a four-probe technique in the range 20-300K.